checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SAlOC-1@G4

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: SAlOC-1@G4

Bond precision: C-C = 0.0121 A   Wavelength=1.34050

Cell: a=30.0800(2)   b=30.0800(2)   c=19.6522(2)
                   alpha=90   beta=90   gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	17781.4(3)	17781.4(3)
Space group	P 4/n	P 4/n
Hall group	-P 4a	-P 4a
Moiety formula	C216 H362 Al32 N12 O110 Pb6 S12, 3(C10 H18 O) [+ solvent]	C216 H362 Al32 N12 O110 Pb6 S12, 3(C10 H18 O)
Sum formula	C246 H416 Al32 N12 O113 Pb6 S12 [+ solvent]	C246 H416 Al32 N12 O113 Pb6 S12
Mr	7841.21	7841.10
Dx,g cm-3	1.464	1.465
Z	2	2
Mu (mm-1)	5.004	5.144
F000	7960.0	7960.0
F000'	7939.61	
h,k,lmax	35,35,23	35,33,23
Nref	15177	15118
Tmin,Tmax		1.000,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=1.000 Tmax=1.000
AbsCorr = SPHERE

Data completeness= 0.996   Theta(max)= 52.047

```
R(reflections)= 0.0481( 12843)                    wR2(reflections)=
                                                  0.1360( 15118)

S = 1.025                    Npar= 976
```

The following ALERTS were generated. Each ALERT has the format
        test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

🔴 Alert level B

```
PLAT220_ALERT_2_B NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range      7.6 Ratio
```

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

```
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of      C27 Check
```

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

```
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of       N2 Check
```

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

🟡 Alert level C

```
RADNW01_ALERT_1_C  The radiation wavelength lies outside the expected range
          for the supplied radiation type. Expected range 1.34130-1.34150
          Wavelength given =    1.34050
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
          Calculated sin(theta_max)/wavelength =    0.5882
PLAT220_ALERT_2_C NonSolvent   Resd 1  O   Ueq(max)/Ueq(min) Range      5.7 Ratio
```

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

```
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range      10.0 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C3 Check
```

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C4 Check
```

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C52 Check
```

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C53 Check
```

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

```
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       N1 Check
```

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

```
PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of        N3 Check
```

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

```
PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of        C2 Check
```

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

```
PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of        C32 Check
```

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

```
PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of        C35 Check
```

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

```
PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of        C41 Check
```

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

```
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      O65      0.193 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............   0.01215 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn      H25B     ..H27B    .      1.81 Ang.
                                             x,y,z  =     1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X       H18     ..H41     .      1.90 Ang.
                                           3/2-y,x,z  =    3_655 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   2.743 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.588      56 Report
            2  2  0,   1  3  0,   3  3  0,   1  5  0,   0  6  0,   0  2  1,
            1  2  1,  -1  3  1,   0  3  1,   0  5  1,   2  5  1,   3  6  1,
            2  9  1,  -7 10  1,  10 13  1,   0  0  2,   0  2  2,  -2  3  2,
            1  3  2,  -1  4  2,   3  4  2,   1  5  2,   3  5  2,   3  6  2,
           -5  7  2,   4  7  2,   1  9  2,   7 11  2,   7 13  2,   0  0  3,
            2  5  3,   0  6  3,   4  7  3,   5  7  3,  -2 12  3,   3 14  3,
            0  3  4,   3  3  4,   4  4  4,  -1  6  4,   2  6  4,  -4 12  4,
           -2 12  4,  -4  5  5,  -4  7  5,   3  5  6,   2  6  6,   5  6  6,
           -7  9  6,   1  9  6,  11 15  6,   4  8  7,   0 10  7,   8 10  7,
           16 18 11,  17 19 11,
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on      Pb3      1.46 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on      Pb2      1.39 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on      Pb1      1.01 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  1.05Ang From O25    .     -0.44 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H18      .     -0.39 eA-3
```

⬤ **Alert level G**

```
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
               not performed for this radiation type.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite      12 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms       70 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............       3 Report
            H5      H18     H65
PLAT051_ALERT_1_G Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .   2.72 %
PLAT069_ALERT_1_G Atom Label Without Numerical Part ..............    Al Do !
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large  29.55 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records     10 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records      3 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records      3 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records      2 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used  0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used  0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used  0.0010 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar  0.0200 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar  0.0200 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par  0.0010 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar  0.0020 Report
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at .............   0.5 Check
            C6      C7      C55     C56     H5BA    H5BB    H5A     H6A
            H6B     H6C     H7A     H7B     H7C     H54A    H54B    H54C
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                  H54D    H55A    H55B    H55C    H56A    H56B    H56C
PLAT300_ALERT_4_G Atom Site Occupancy of O65        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C30        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C57        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C58        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C59        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C60        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C61        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C62        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C63        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C64        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C66        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H30A       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H30B       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H30C       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H57A       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H57B       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H57C       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H59A       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H59B       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H60A       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H60B       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H61        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H62A       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H62B       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H63        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H65        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H66A       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H66B       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H66C       Constrained at       0.75 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)        2% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    2)      100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    2)    21.75 Check
PLAT343_ALERT_2_G Unusual sp3     Angle Range in Main Residue for       C27 Check
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C4      - C5      .       1.51 Ang.
PLAT410_ALERT_2_G Short Intra H...H Contact  H53A     ..H54B   .       2.05 Ang.
                                            x,y,z  =      1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H53B     ..H54A   .       2.05 Ang.
                                            x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H51B     ..H56B   .       2.03 Ang.
                                            x,y,z  =      1_555 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H1C      ..H6B    .       1.82 Ang.
                                           1/2+y,1-x,1-z  =      7_666 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H29A     ..H56C   .       1.87 Ang.
                                           -1/2+y,1-x,1-z  =      7_566 Check
PLAT415_ALERT_2_G Short Inter D-H..H-X       H26A     ..H65    .       1.87 Ang.
                                           -1/2+y,1-x,1-z  =      7_566 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O65      ..C26    .       3.00 Ang.
                                           1-y,1/2+x,1-z  =      8_666 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure      98 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       3 Note
             Al00    H5BA    H5BB
PLAT793_ALERT_4_G Model has Chirality at C61       (Centro SpGr)        S Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1        (II)     .     2.09 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb3        (II)     .     2.03 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al00       (III)    .     2.74 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al2        (III)    .     2.81 Info
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PLAT794_ALERT_5_G Tentative Bond Valency for Al3         (III)     .       2.82 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al4         (III)     .       2.75 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al5         (III)     .       2.80 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al6         (III)     .       2.82 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters        6 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      469 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed        ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .   Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still      67% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).        3 Note
          1  1  0,   0  0  1,   0  1  1,
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....        1 Note
          1  1  0,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File       53 Note
          3  6  1,   2  2  0,   2  6  4,   8 10  7,   1  9  2,   7 13  2,
          2  6  6,   3  3  4,   2  5  3,   0  6  3,  -4 12  4,   4  7  2,
          2  9  1,   4  7  3,   4  4  4,   1  9  6,   0  2  1,  -5  7  2,
         -4  5  5,   0  3  4,  -2 12  4,  10 13  1,   3 14  3,  -1  4  2,
          3  4  2,   3  6  2,   3  5  2,   0 10  7,  -2  3  2,   5  7  3,
          7 11  2,  11 15  6,  -1  6  4,  -4  7  5,   3  5  6,   5  6  6,
         -2 12  3,   4  8  7,  -7  9  6,   1  3  0,   1  5  2,   1  5  0,
          3  3  0,   1  2  1,   0  2  2,   1  3  2,   0  5  1,   0  6  0,
          0  3  1,  -7 10  1,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........      3.3 Low
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ         2 Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........    3.597 Note
           Predicted wR2: Based on SigI**2  3.78 or SHELX Weight 13.28
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        0 Info
PLAT984_ALERT_1_G The   C-f'=    0.0147 Deviates from the B&C-Value    0.0137 Check
PLAT984_ALERT_1_G The   N-f'=    0.0253 Deviates from the B&C-Value    0.0241 Check
PLAT984_ALERT_1_G The   O-f'=    0.0412 Deviates from the B&C-Value    0.0389 Check
PLAT984_ALERT_1_G The Pb-f'=   -4.2646 Deviates from the B&C-Value   -4.4950 Check
PLAT985_ALERT_1_G The Al-f"=    0.1843 Deviates from the B&C-Value    0.1873 Check
PLAT985_ALERT_1_G The Pb-f"=    7.1982 Deviates from the B&C-Value    6.8412 Check
PLAT985_ALERT_1_G The  S-f"=    0.4242 Deviates from the B&C-Value    0.4295 Check
```

```
  0 ALERT level A = Most likely a serious problem - resolve or explain
  3 ALERT level B = A potentially serious problem, consider carefully
 25 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 90 ALERT level G = General information/check it is not something unexpected

 12 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 36 ALERT type 2 Indicator that the structure model may be wrong or deficient
 18 ALERT type 3 Indicator that the structure quality may be low
 41 ALERT type 4 Improvement, methodology, query or suggestion
 11 ALERT type 5 Informative message, check
```

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checkCIF publication errors

🔴 Alert level A

PUBL004_ALERT_1_A The contact author's name and address are missing,
        _publ_contact_author_name and _publ_contact_author_address.

```
PUBL005_ALERT_1_A  _publ_contact_author_email, _publ_contact_author_fax and
               _publ_contact_author_phone are all missing.
               At least one of these should be present.
PUBL006_ALERT_1_A  _publ_requested_journal is missing
               e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A  _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A  _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A  _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A  _publ_section_abstract is missing.
               Abstract of paper in English.
```

```
   7 ALERT level A = Data missing that is essential or data in wrong format
   0 ALERT level G = General alerts. Data that may be required is missing
```

Publication of your CIF

You should attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. *checkCIF* was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
```

```
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 15/07/2024; check.def file version of 15/07/2024

NOMOVE FORCED

Prob = 50
Temp = 100

Y
-8

PLATON-Aug 1 13:46:37 2024 - (150724)

Z -42   SALOC-1@G4   P 4/n   R = 0.05   RES= 0   -8 X